The role of high performance computing in predictive models for microstructure evolution of irradiated Fe and FeCr alloys

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1st Spanish Fusion HPC Workshop , November 27, 2020 (Zoom meeting, BSC)

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Experiments:

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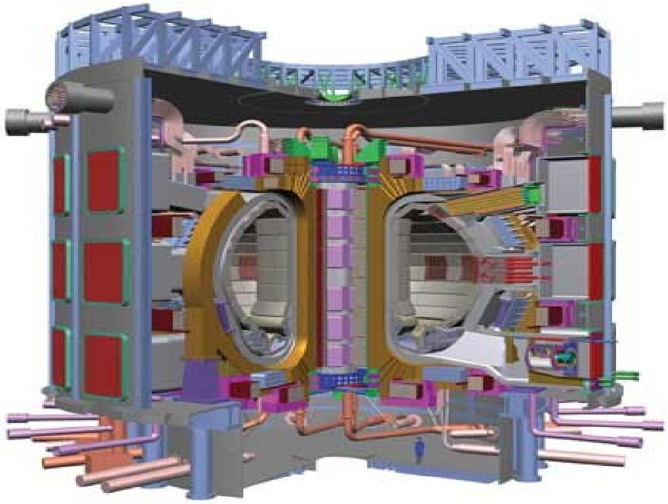
R. Schaeublin, ETH-Zurich (Switzerland), Anna Prokhodtseva

Outline

- Multiscale modeling of materials, why?
- Simulation methods and experimental validation.
- Initial damage: molecular dynamics simulations.
- Modeling microstructure evolution: kinetic Monte Carlo
- Conclusions

Materials: one of the main challenges of fusion

The next step in magnetic fusion: **ITER**
(International Tokamak Experiental Reactor)



EUROfusion

Roadmap

Theory and modelling effort in plasma and material physics is crucial.

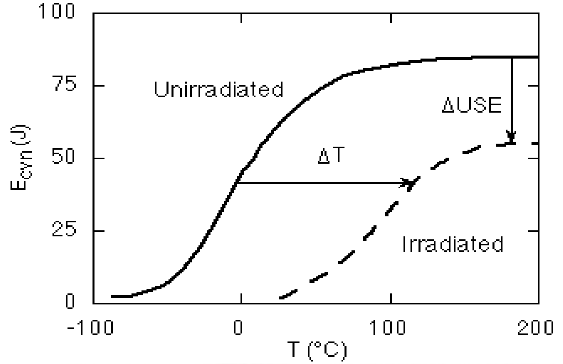
Exposure to radiation changes the mechanical behaviour of materials

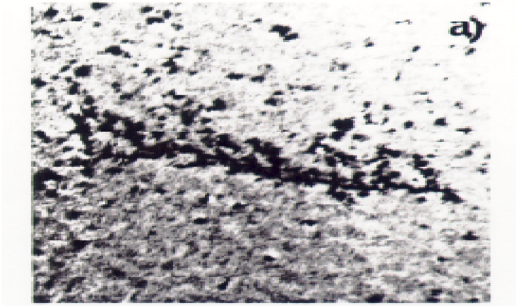
Exposure of metals to high-energy particle irradiation produces significant microstructural changes and dramatically alters mechanical properties

Macroscopic

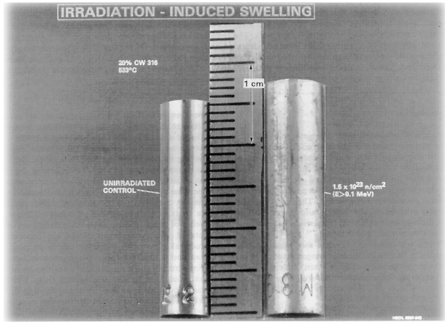
Microscopic

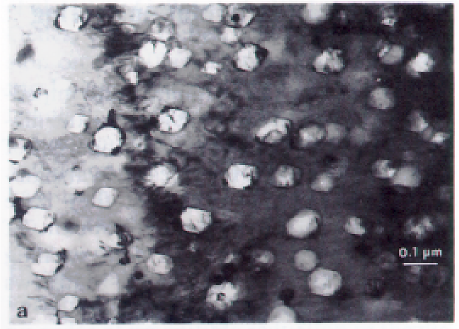
Embrittlement



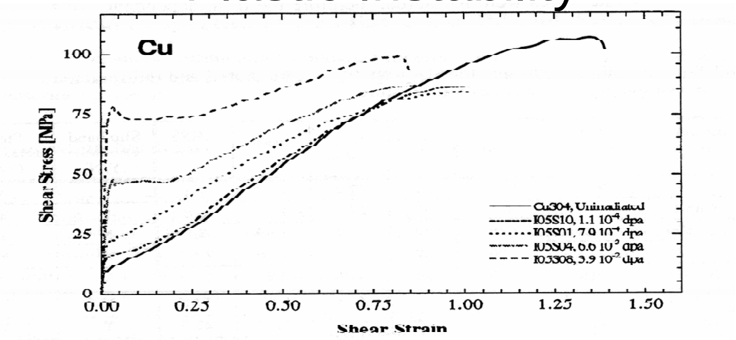


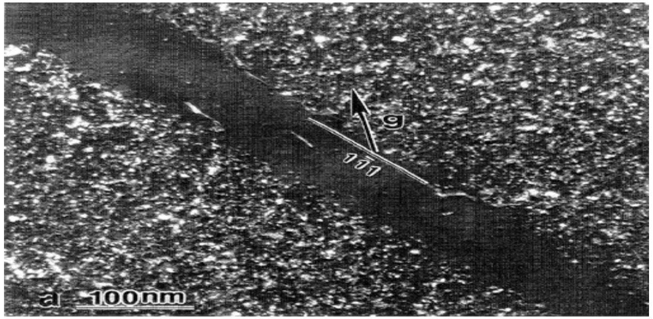
Swelling





Plastic Instability





Need to understand microscopic processes to predict macroscopic properties

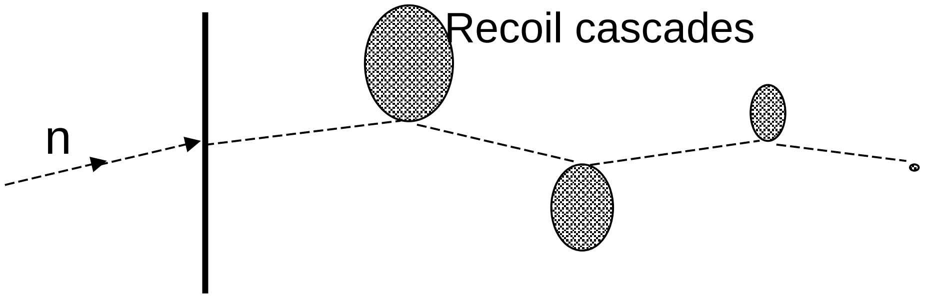
Why do we need modelling?

- More efficient selection of materials
- Predict the behaviour of materials under different conditions (irradiation, temperature, time ...)
- Link between different type of irradiation: neutron vs. Ion

Only possible if we know the fundamental processes that occur during irradiation and their time evolution

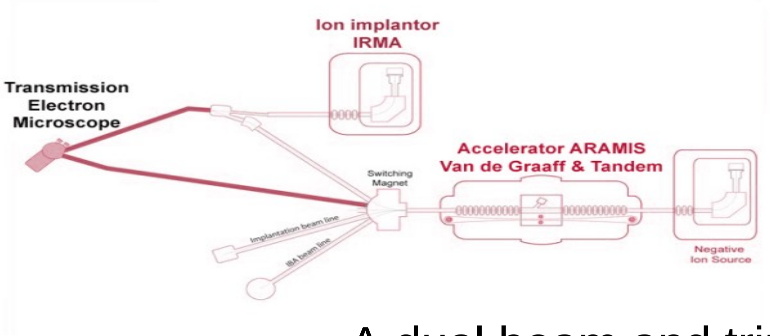
Models to extrapolate from ion irradiation to neutron damage

Need to understand neutron damage of ~ MeV range
production of recoils of 10s of keVs



Neutron experiments
difficult/costly/limited

Use of ion irradiation to understand defect production and defect evolution



JANNUS

A dual beam and triple beam facility at CEA, France

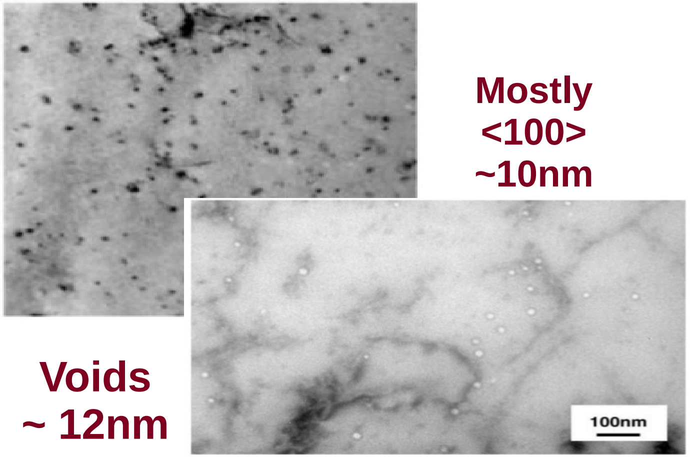
http://jannus.in2p3.fr/

Model validation with ion irradiation - extrapolation to neutrons

Microstructure varies significantly with irradiation conditions even in pure Fe

M. Hernández-Mayoral et al, JNM (2010) 146

Neutron irradiation 0.19 dpa T = 300^{o}C



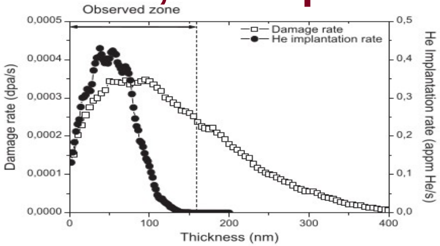
Mostly <100> ~10nm

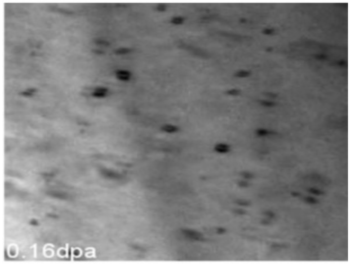
Voids ~ 12nm

Brimbal et al, Acta Mat. 64 (2014) 391 & Acta Mat. 61 (2014) 34757

Ion irradiation T = 500^{o}C

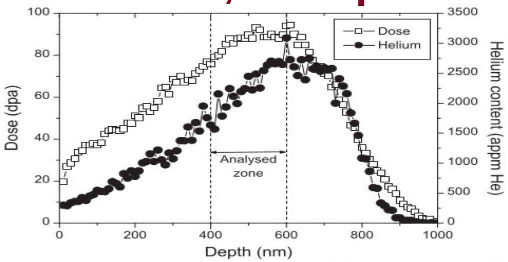
1 MeV, 0.16 dpa



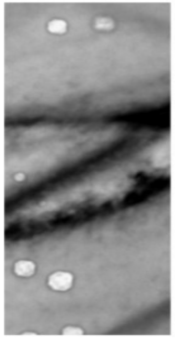


<100> No voids

2 MeV Fe, 100 dpa

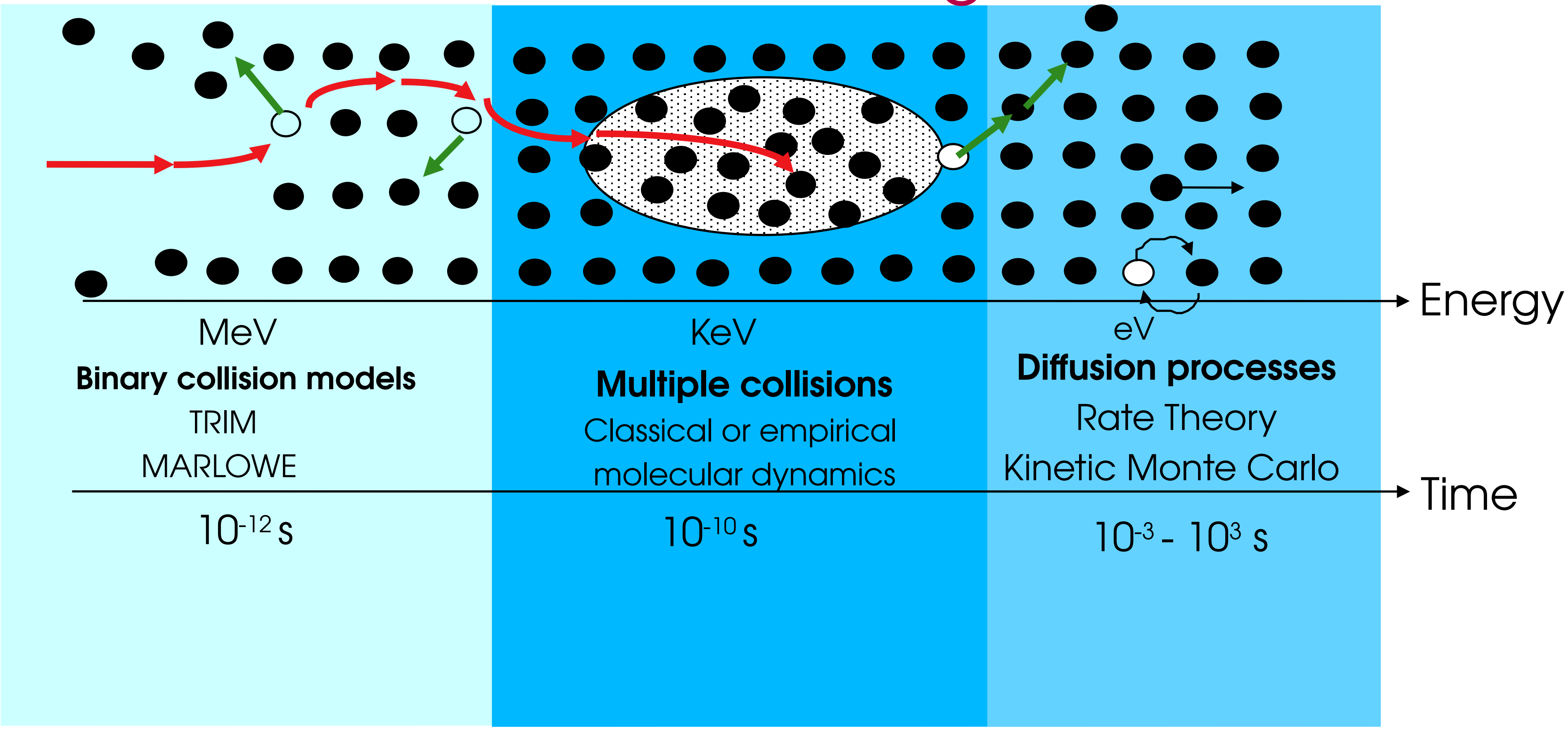


Voids ~ 24 nm Small number of loops Coarse dislocation network



Vast information coming from experiments with different irradiation conditions – methodology for proper comparison

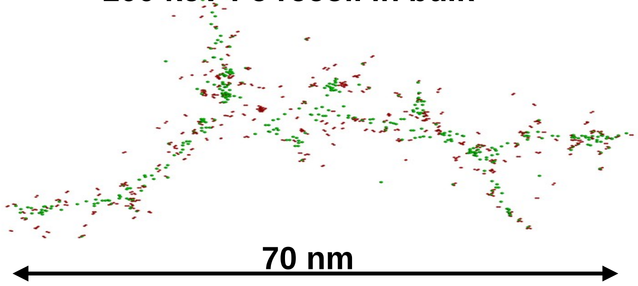
Multiscale modeling is needed to understand radiation damage



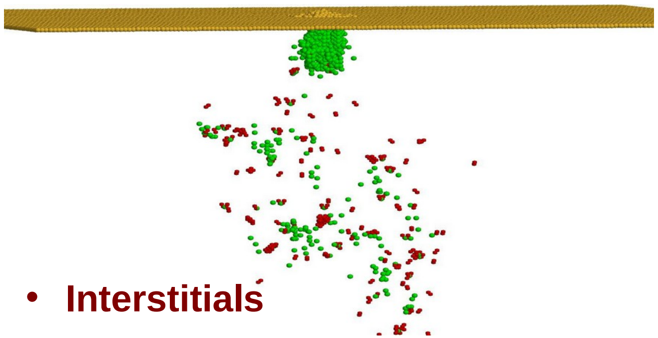
Linking simulation methods to expand time and length scales

MD + DFT → OKMC → Exp

100 keV Fe recoil in bulk

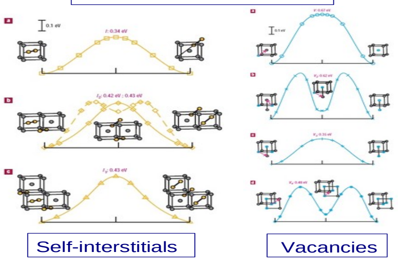


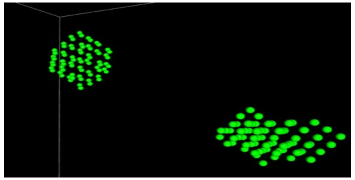
100 keV Fe recoil in thin film

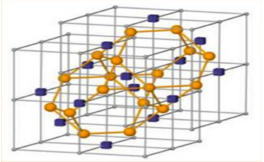


- Interstitials
- Vacancies

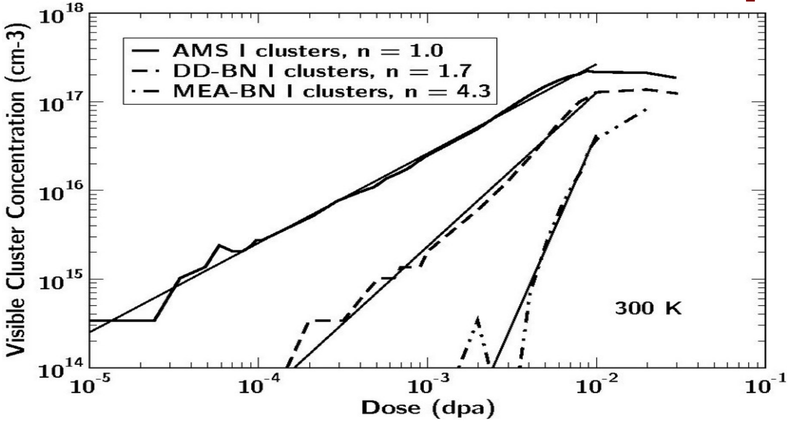
C. C. Fu et al.
Nature Mat. (2004)

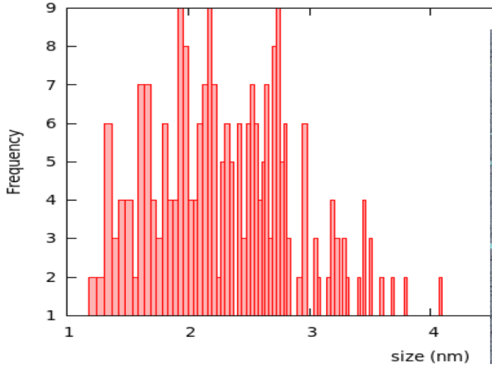


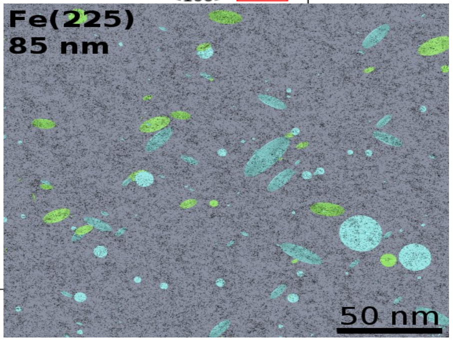




Marinica PRL (2012)



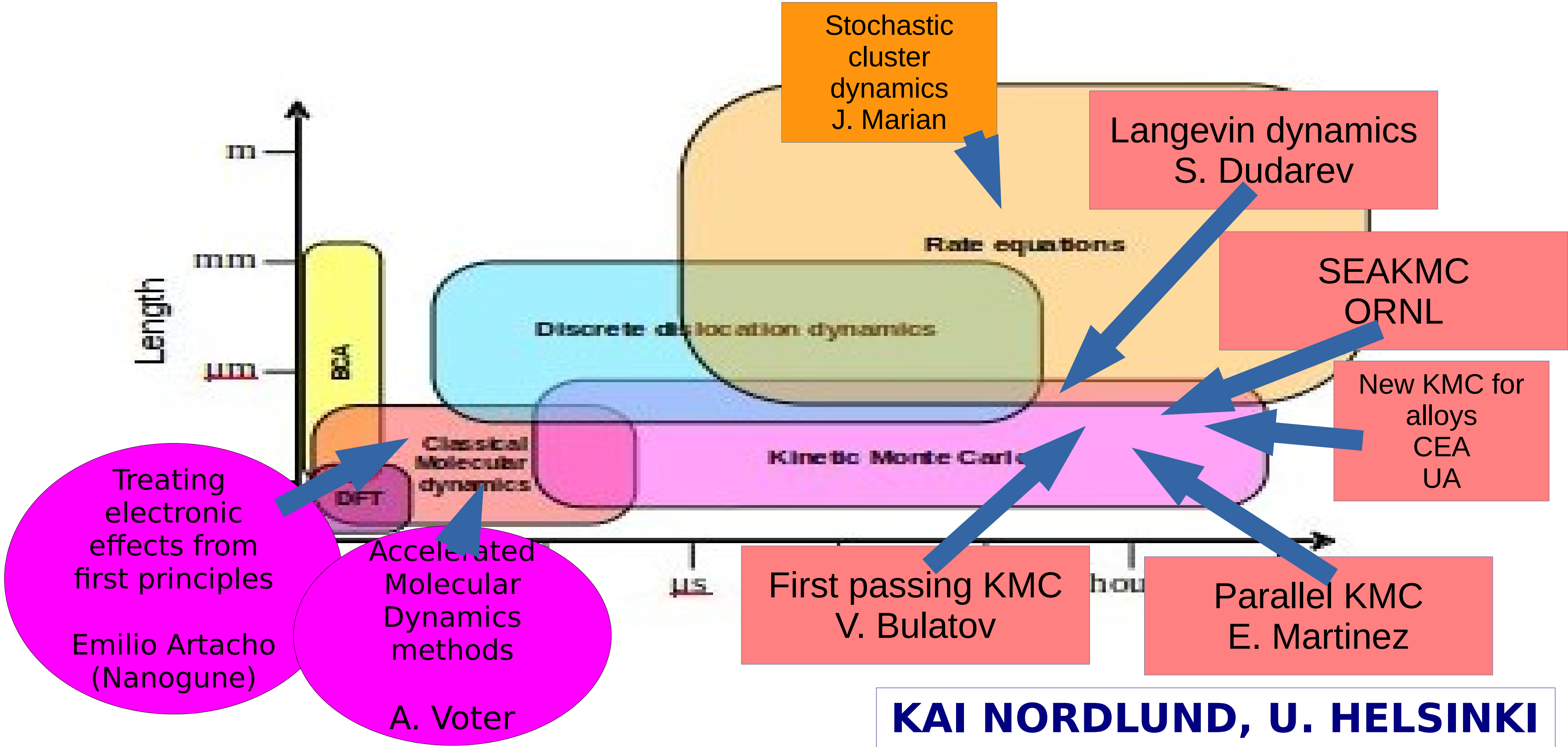




Simulation methods: capabilities and limitations

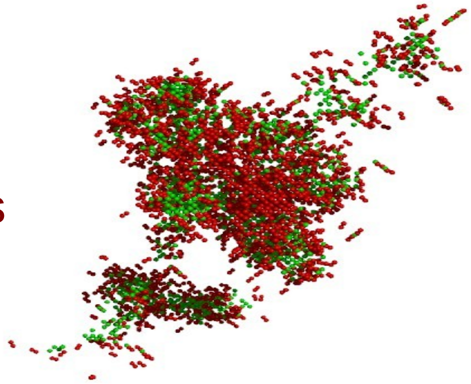
Method	Approximation	Atoms	Upper Size limit	Time
Ab initio - DFT	E. Schrödinger through approx.	All	A few hundred atoms	Static Car-Parinello << ns
Tight-binding	Repulsion - empirical	All	A few thousand atoms	< ns
Classical Molecular Dynamics	Empirical potentials	All	Millions of atoms ~ $(100nm)^3$	~ ns
Kinetic Monte Carlo	Probabilities of events	Only defects	~ $(1000nm)^3$	Hours - years
Rate theory	Mean field	Only defects	No limitations	Hours - years
Dislocation dynamics	Elasticity + short range rules	Only dislocations	~ $(1000nm)^3$	----
Finite elements	Constitutive equations	System is discretized	-----	-----

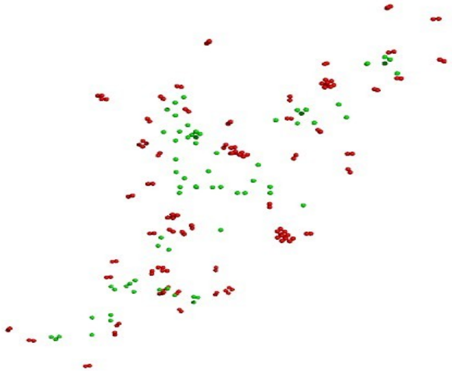
Broad range of new methods being developed



Primary damage: vacancies and self-interstitials - Molecular Dynamics

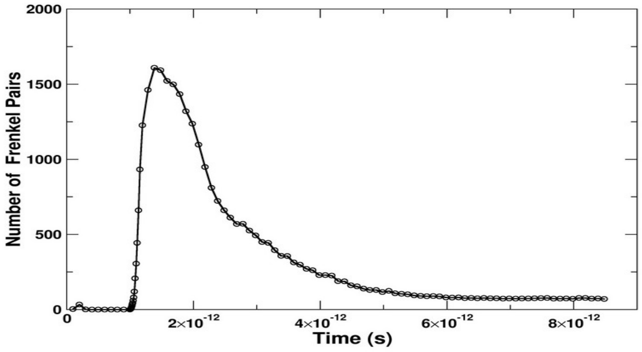
- Vacancies
- Self-interstitials





Show movie 30KeV Cu

Show movie 100 keV Cu



Collision cascade time

~ 10^{-11} s

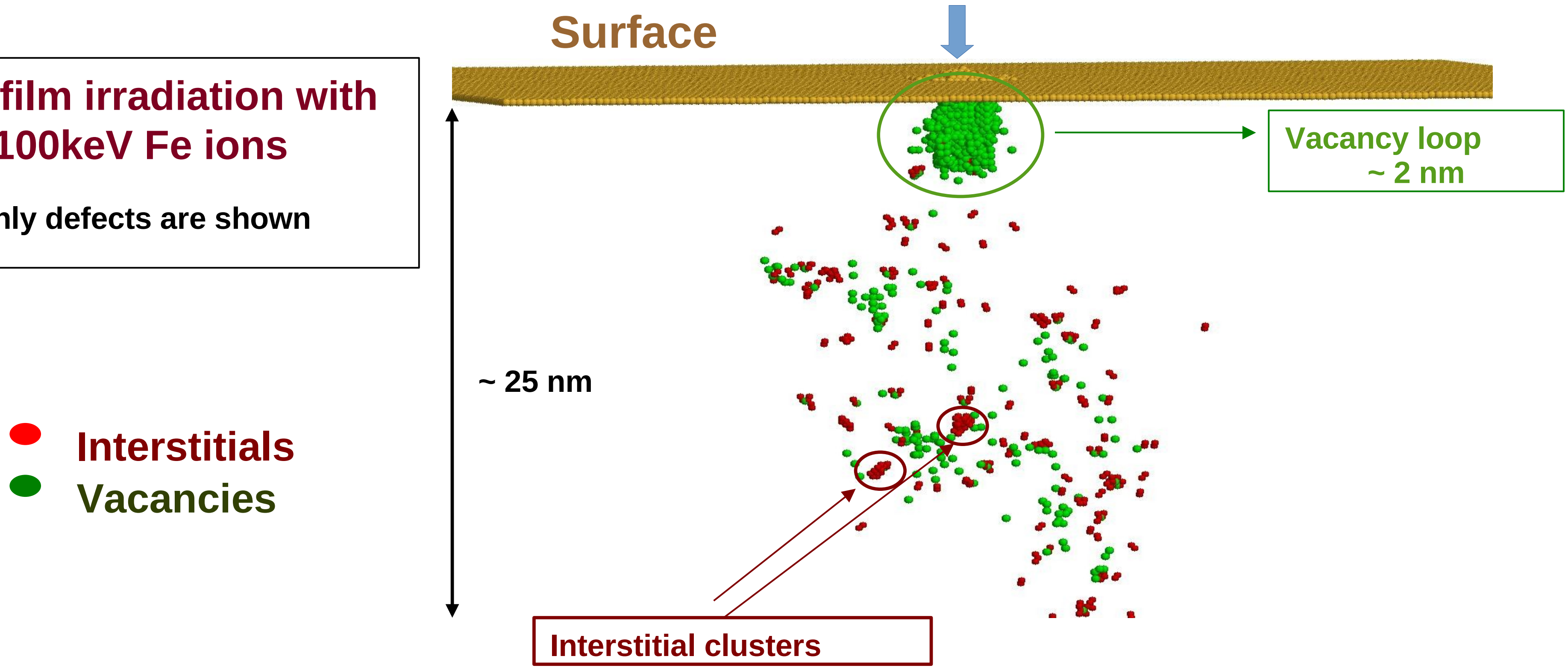
size

~ $(50nm)^3$

Primary damage: surface effects

Thin film irradiation with 100keV Fe ions

Only defects are shown



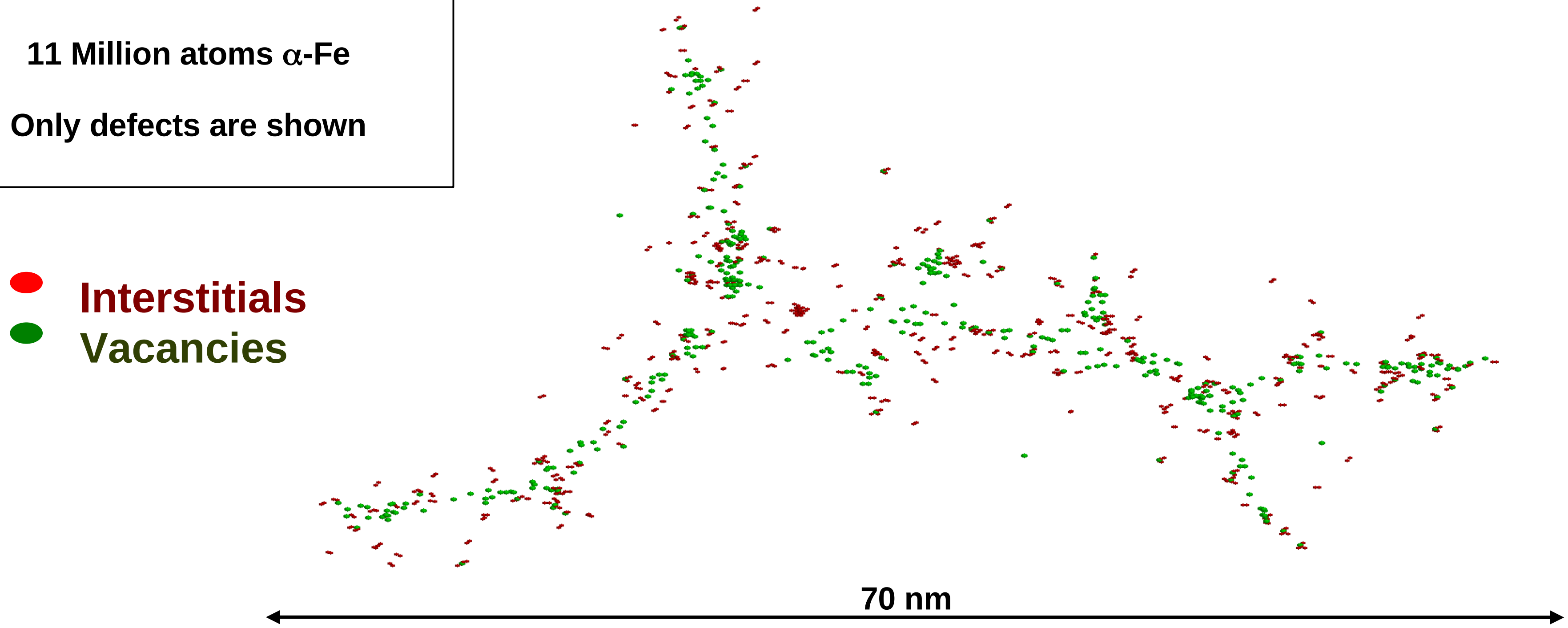
M. J. Aliaga, et. al, Acta Mat. (2015)

Primary damage: bulk damage

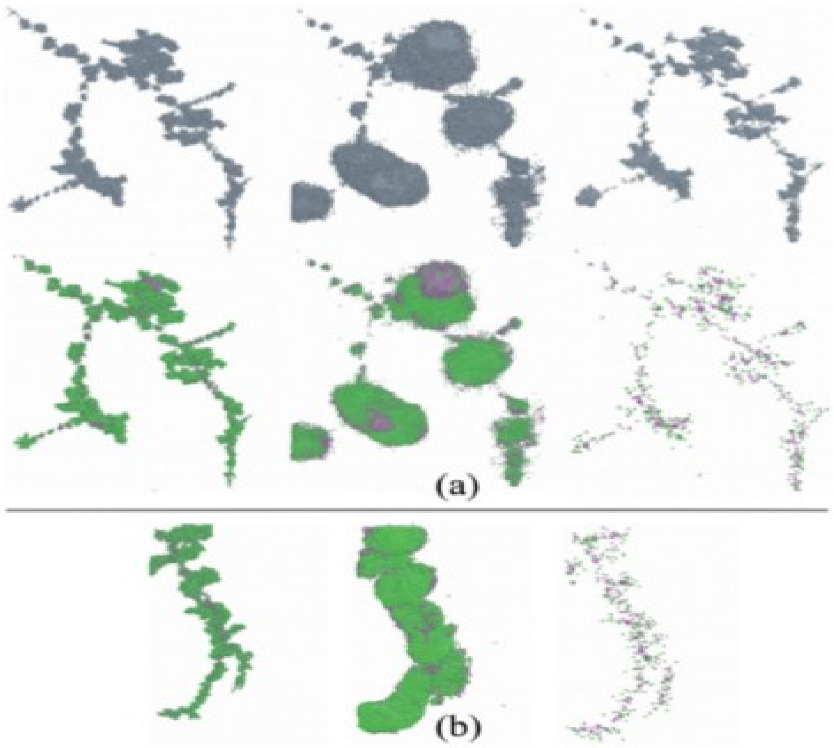
100 keV Fe recoil in bulk

11 Million atoms α-Fe

Only defects are shown



Do these mechanisms add up? 1 + 1 = 2 ?

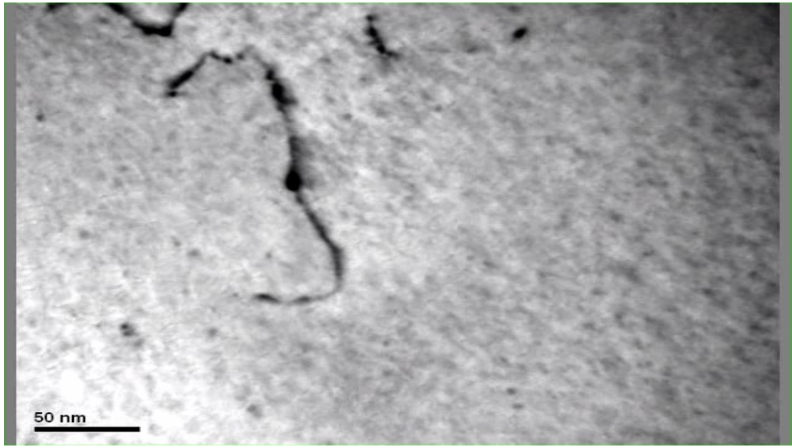


500 kev cascade in Fe

E. Zarkadoula et al,
J. Phys. Condense. Matter 25 (2013) 125402

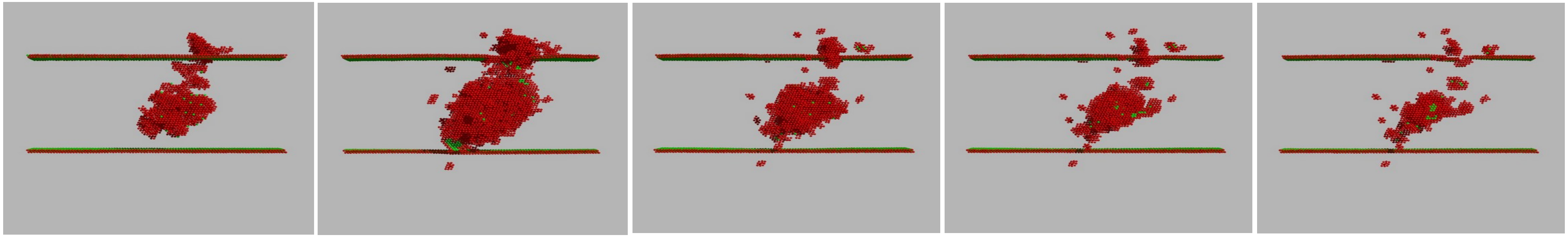
In-situ TEM observations of ion irradiated Fe and FeCr

Experiments by A. Prokhodtseva and R. Schäublin performed at Jannus

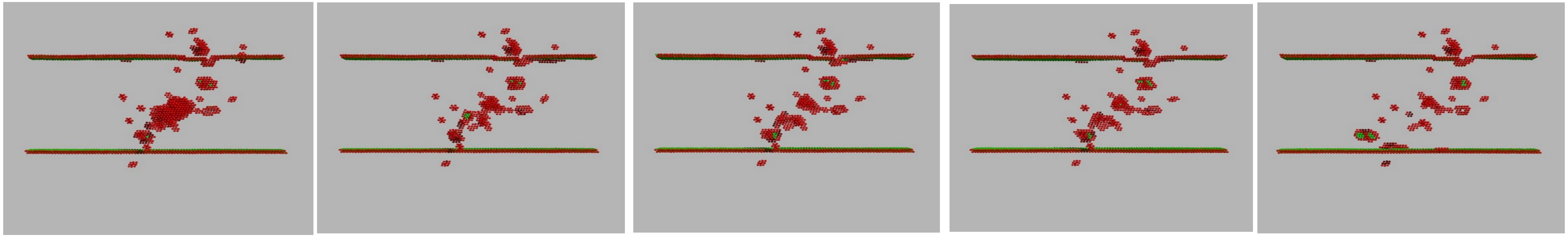


What are the main mechanisms?
Need to understand the interaction between defects and dislocations

Simulation of f.c.c Cu cascades next to dislocations



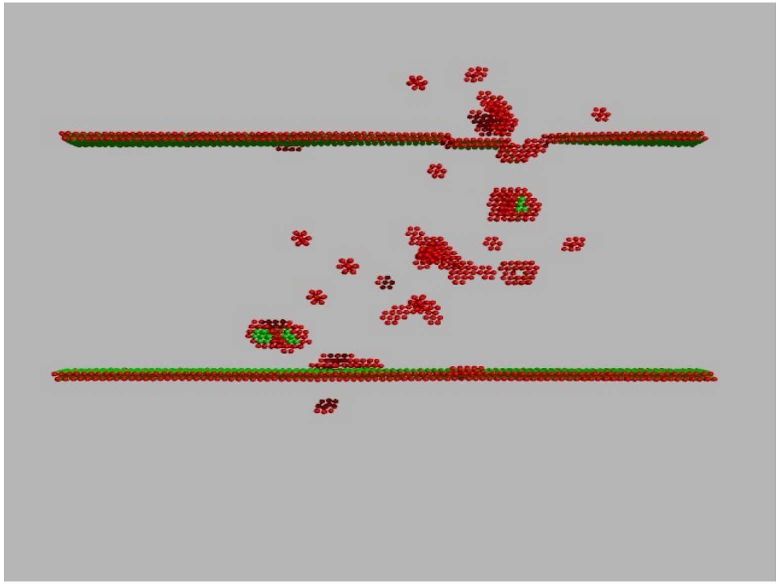
1ps 2ps 4ps 5ps 6ps



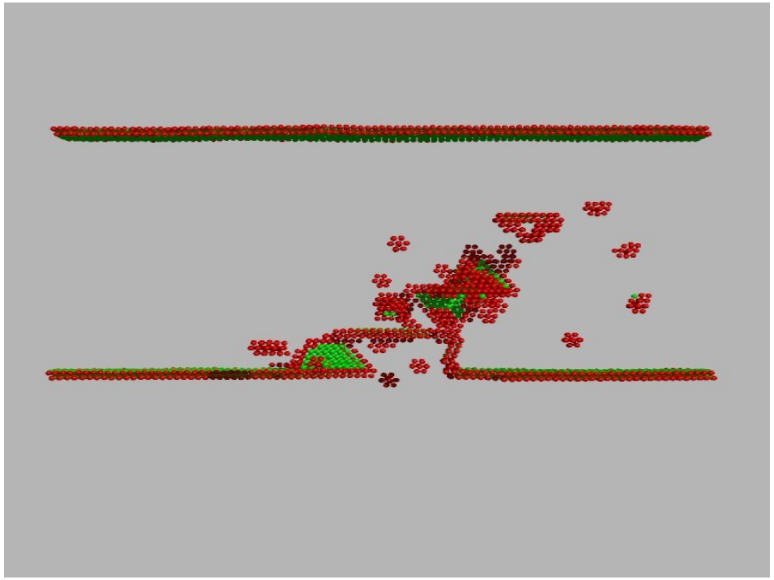
7ps 8ps 9ps 10ps 74ps

Simulation of f.c.c Cu cascades next to dislocations

Case 1

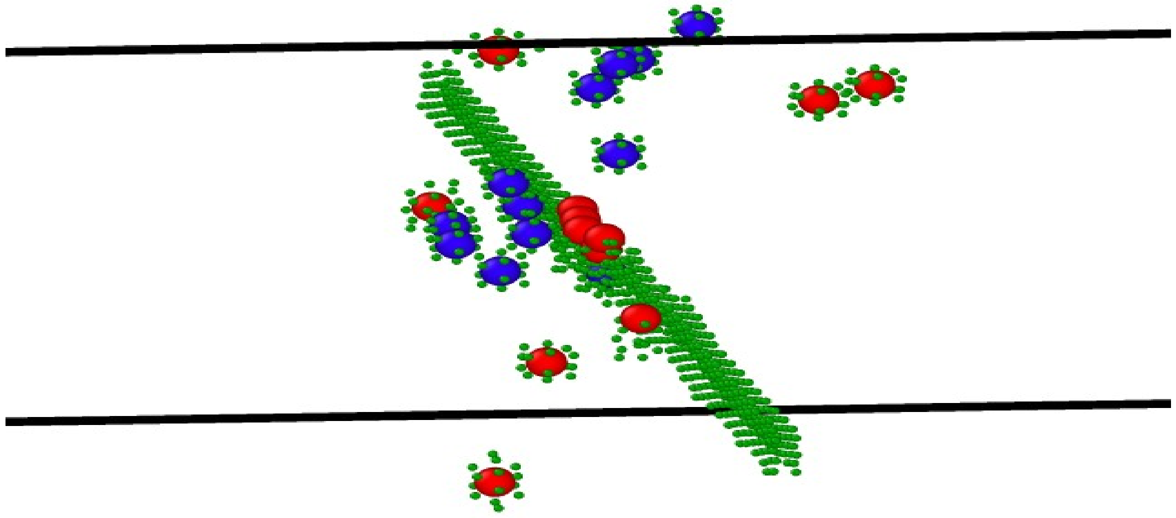


Case 2



Radiation induces changes in dislocation structure
Stacking fault tetrahedron and partial dislocations

Example: edge dipole in b.c.c. Fe
2 keV cascade close to one of the dipoles, T = 20 K

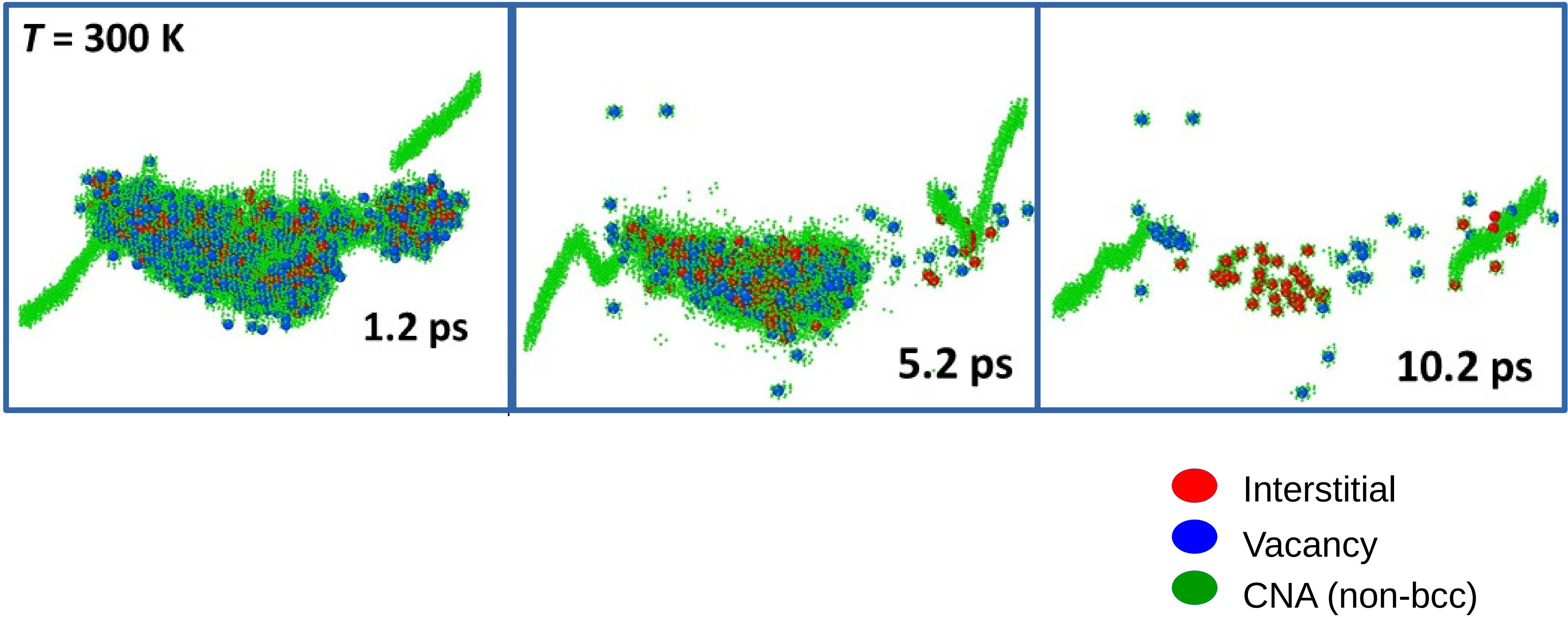


Interstitial
Vacancy
CNA (non-bcc)

Defects after cascade:

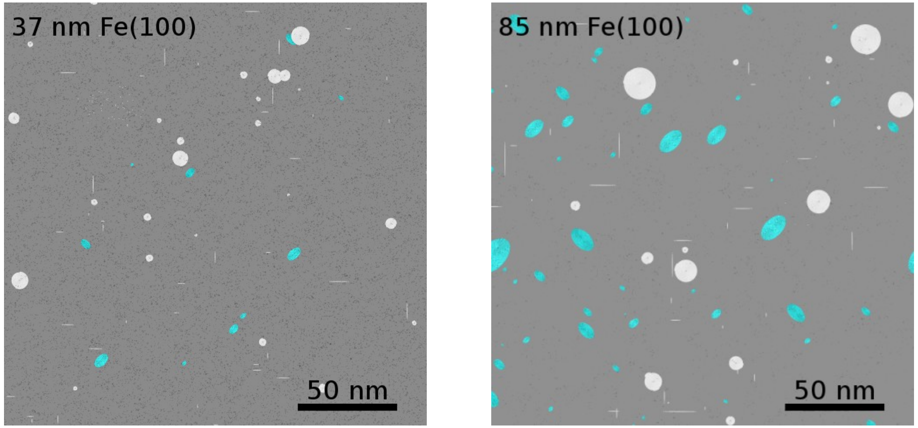
At the dislocation line - 6 interstitials and 1 vacancy
Away from the dislocation – 6 interstitials and 11 vacancies

Example: edge dipole in b.c.c. Fe
20 keV cascade T = 300 K



S. Heredia, et. al, J. Nucl. Mat. (2020)

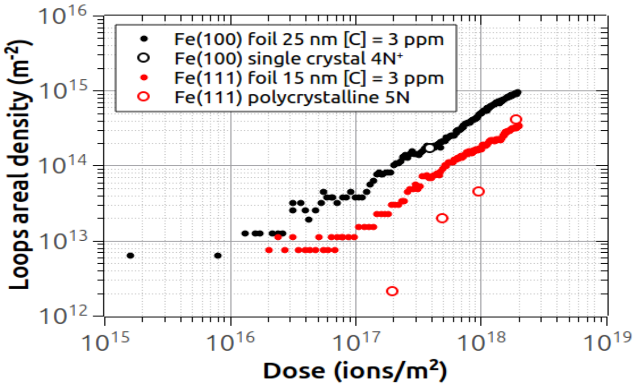
Comparison to experiments: kinetic Monte Carlo



<100> loops

½ <111> loops

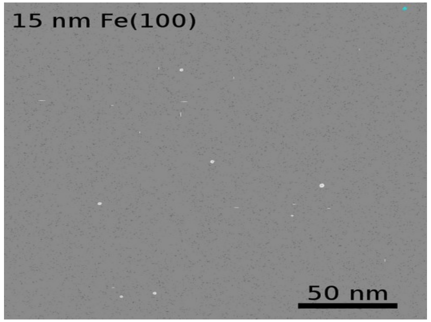
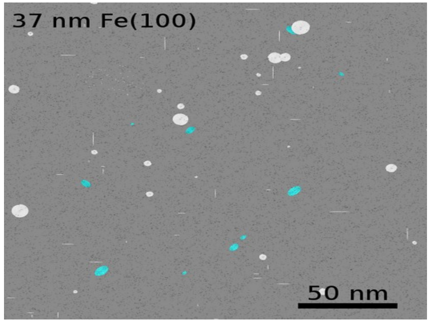
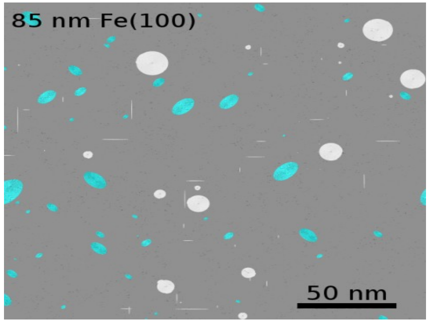
Comparison with experimental data

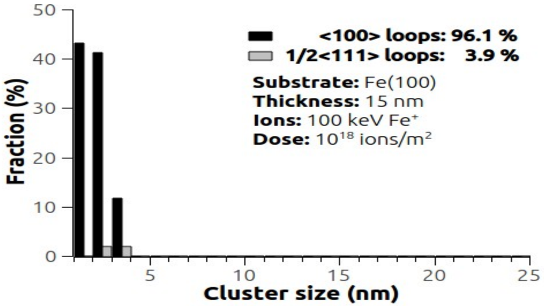


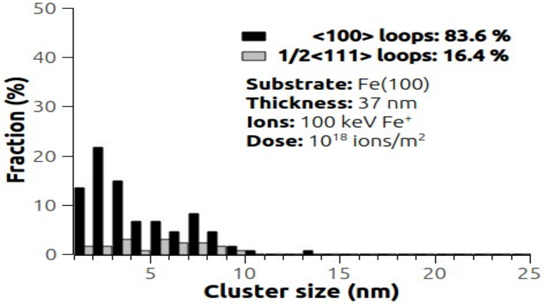
Visibility threshold
~ 1.5nm (30 SIA)
[Yao et al, Phil. Mag. 88 (2008)]

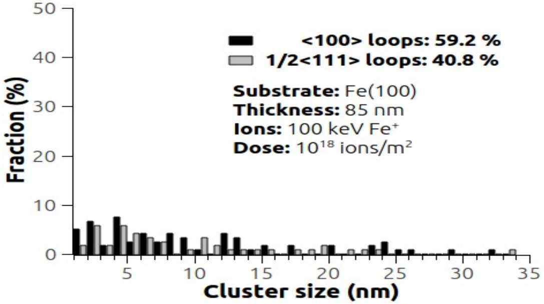
J. P. Balbuena, et. al, JNM (2019)

Dependence on sample thickness and orientation

Sample thickness	15 nm	37 nm	85 nm
Orientation (100)			





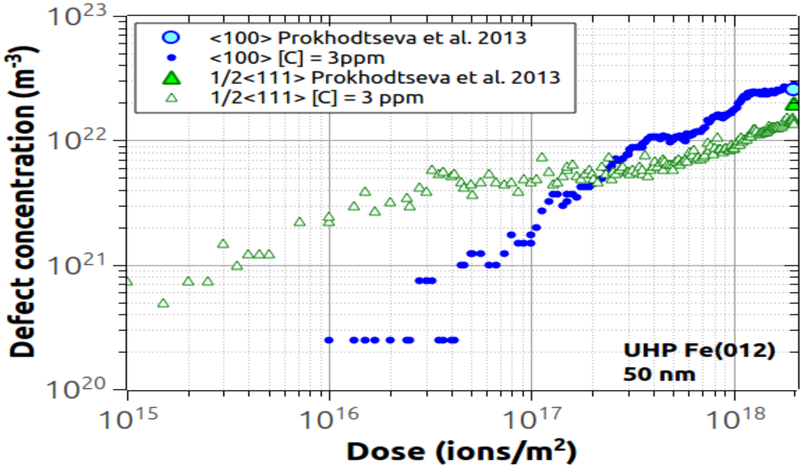


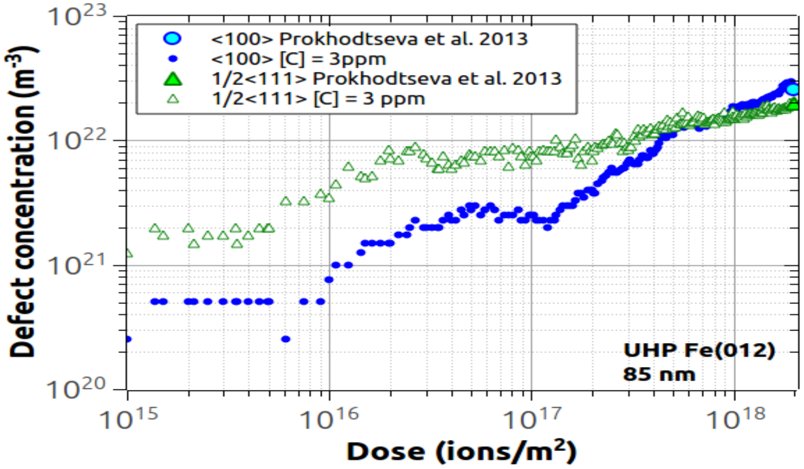
Average size increases with increasing foil thickness

J. P. Balbuena, et. al, JNM (2019)

Increasing the energy of the implanted ion – 0.5 MeV

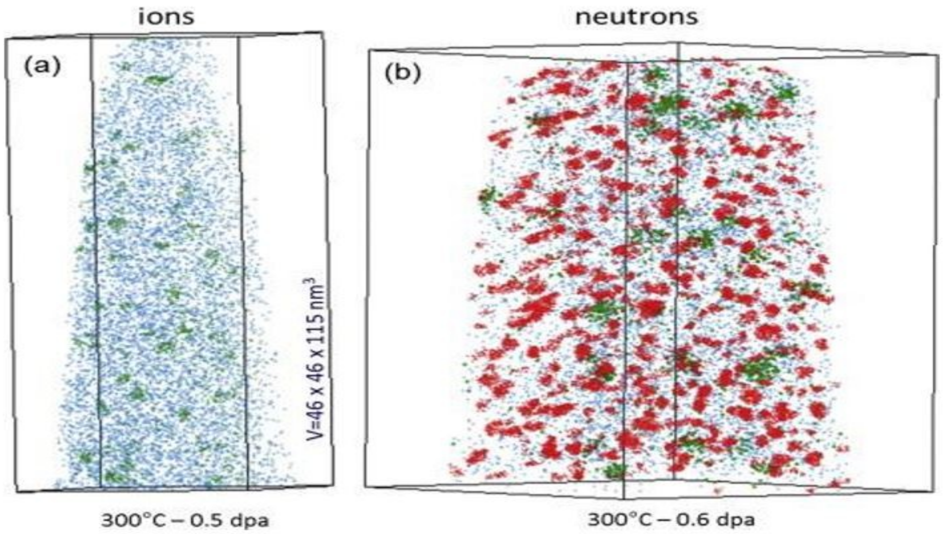
Substrate: Fe(012) 50-85 nm **Temperature:** 294.15 K **Dose rate:** $5x10^{14}$ ions/m^2s





- **High concentration of small ½ <111> loops at early stages of irradiation, for all cases**
- **Higher concentration of ½<111> loops found in thicker foils at intermediate doses**
- **Higher concentrations of <100> loops at the highest dose (1 dpa) for all cases**

Complex chemistry: FeCr alloys as well as impurities



P
Si
XCr > 28%

APT Fe-12Cr 300°C
(a) ion 0.5 dpa (b) neutron 0.6 dpa

C. Pareige et al. JNM 456 (2015) 471–476

Atom Probe Tomography (APT)

Modeling with kinetic Monte Carlo requires a large parameter data set

Conclusions

- Large scale molecular dynamics simulations of collision cascades needed to understand initial damage production
- Simulations in the presence of dislocations less explored but provide relevant information about microstructure evolution in irradiated materials
- Microstructure evolution over relevant time scale require other methods such as OKMC
- Efficient methods to improve parameters in these OKMC models – artificial inteligence

Acknowledgments - funding

This work has been carried out within the framework of the EUROfusion Consortium and has received funding from the Euratom research and training programme 2014–2018 and 2019–2020 under grant agreement No 633053.

The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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